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Modeling and Simulation Framework for Advanced Fuel Cycles

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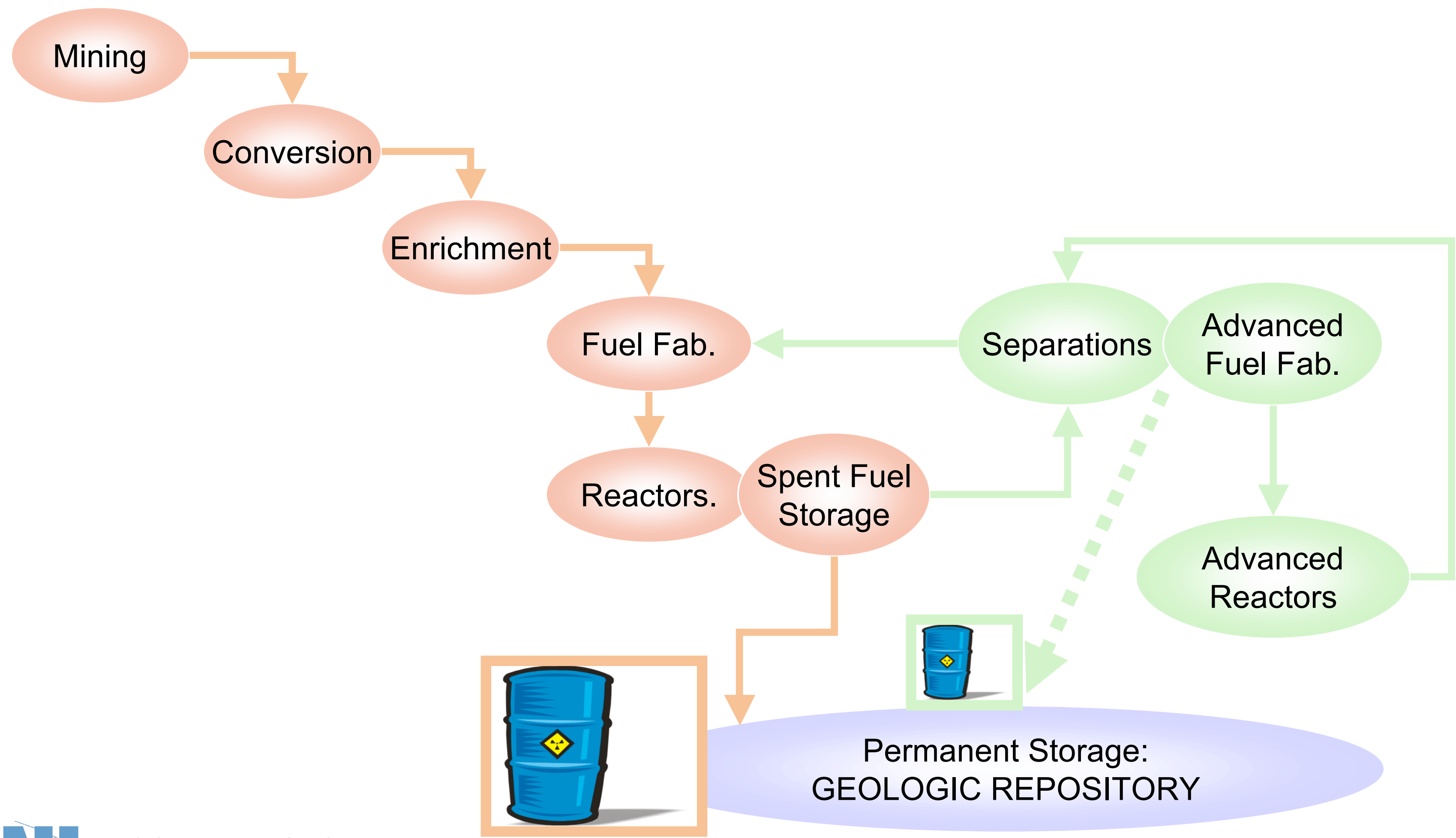
Implementation of advanced fuel cycles requires detailed understanding of interactions among various complex technologies



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Development of the future nuclear energy enterprise must take full-advantage of advanced modeling and simulation capabilities.

- Nuclear energy systems and associated enterprise are complex.
  - A detailed understanding of technical, economic, political, social and environmental issues is required.
  - National interests must be balanced against International concerns
- Operating and maintaining the nuclear research facilities are expensive
  - Development of progressive advanced fuel cycles by empirical means only is cost prohibitive
  - In the U.S. most facilities are shut down and International facilities are not adequate to support a rapid growth
  - Additional facilities must be targeted on the most promising nuclear energy future.
- Advanced computing and simulation have made remarkable progress
  - Most tools used in nuclear industry are 20+ years old
  - Computing power has grown and continue to grow exponentially
  - Other fields are extensively using the new capabilities (e.g. aircraft design)
  - “Virtual” problem solving networks are becoming standard practice in other industries

A "computational interactive tool-box" tailored to the needs of a wide-variety of potential users is possible

- Provide high fidelity dynamic simulation of fuel cycles
  - Assess technology implications on
    - Economics & sustainability
    - Safety and environmental issues
    - Proliferation & International relations
  - Provide technical input to decision makers
- Reduce cost of nuclear energy
  - New tools for developing and designing innovative technologies
  - Shorten the development and deployment time by optimizing systems in a computational domain first
  - Reduce uncertainty and R&D cost by reducing the number of expensive large scale experiments
  - Perform virtual experiments when physical experiments are too expensive or impossible
- Guide the rebuilding of the research infrastructure
  - Define experimental data needs and design facilities
  - Built facilities to support the most promising future technologies
  - Establish a common protocol for data collection, analyses and archiving
  - Establish joint university-national laboratory-industry-regulatory agency research projects

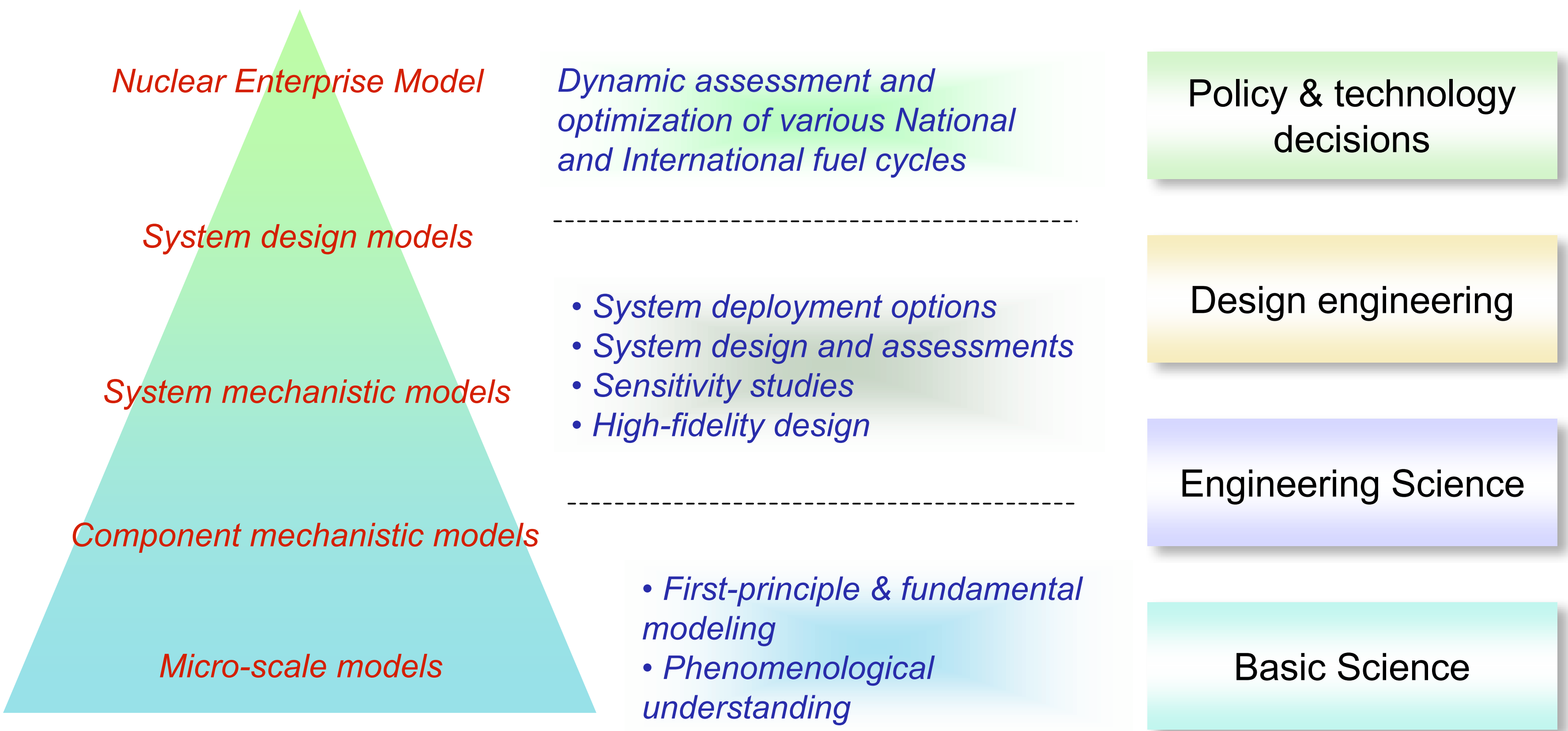
<u>Advanced visualization</u>
• Walk-through models
• Numerical prototyping
• Easy I/O processing

<u>High-fidelity mechanistic models</u>
• Fundamental - first principle models
• Virtual experiments
• Design optimization
• Simpler-cheaper experiments

<u>Fully interactive models</u>
• Coupled phenomenology
• Multi-scale (spatial & temporal), multi-attribute analyses.
• Dominant phenomena

<u>High-speed computation</u>
• Realistic assessment of options
• Tool for decision-makers

A multi-tier, multi-scale and multi-purpose simulation and modeling strategy is possible using the integrated toolbox



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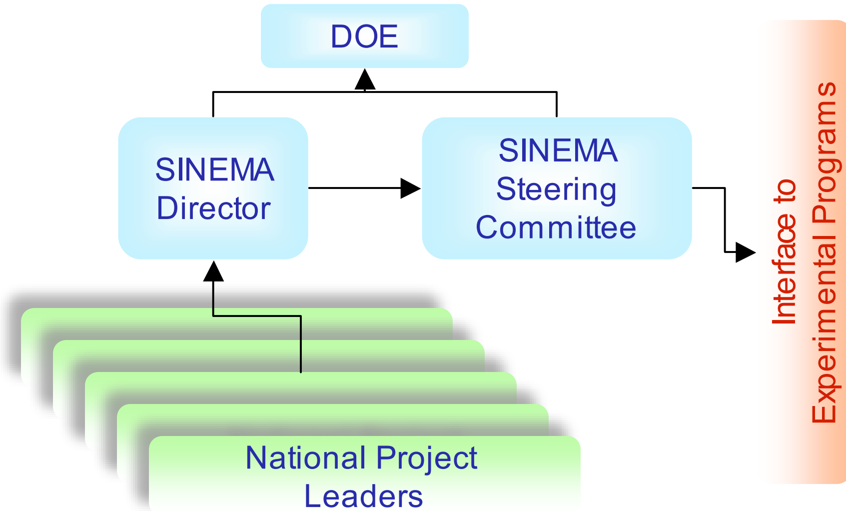
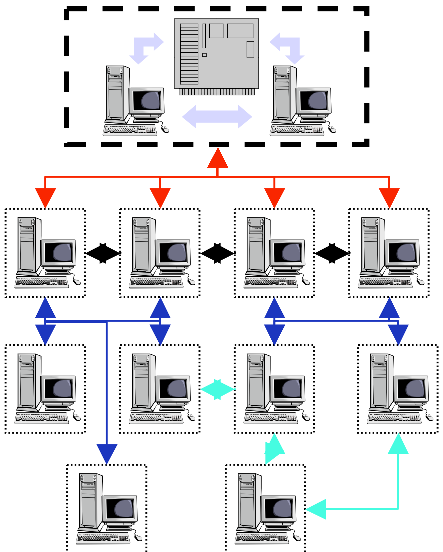
A National framework for the "toolbox" has been proposed: Simulation Institute for Nuclear Enterprise Modeling and Analysis (SINEMA)

- SINEMA can be formed as an institute at a National Laboratory (e.g. INL) and can be administered by an Institute Director
  - A national management structure will be developed, using expertise at other sites for project leads.
- A National Steering Committee must be established to guide and monitor the performance.
- The SINEMA computational network should be centered at the Institute





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FUEL CYCLE TECHNOLOGIES

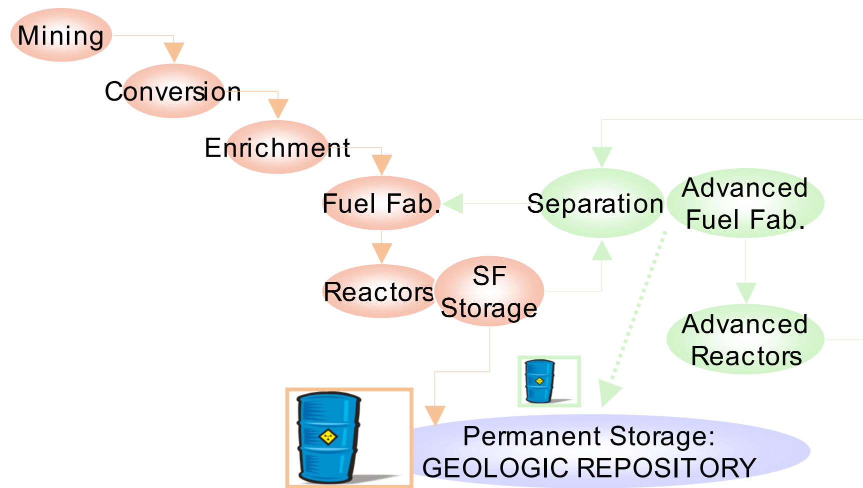
- Mining, milling, conversion
- Enrichment
- Fuel fabrication
- Separations
- Reactors
- Transmuters
- Temporary storage
- Permanent storage

CROSS-CUTTING TECHNOLOGIES

- Networking and hardware
- Software engineering
- Validation & verification
- Proliferation assessment
- Economic assessment
- Safety assessment
- Environmental assessment
- Transportation

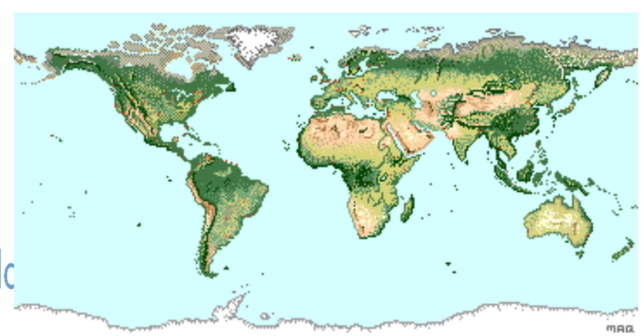
The nuclear enterprise model can be built using the existing codes with needed improvements

- Propagation of uncertainties through the entire system
  - Scientific uncertainties
  - Modeling biases
  - Technology confidence levels
- System level optimization
  - Scenario assessment versus optimization with multiple objectives
- Discrete tracking of materials
  - Preserving materials history
  - Optimizing blending schemes
- Fully-modular approach with capability to use
  - Diverse plants
  - Diverse technologies
- Visual I/O interface
  - Tailored to user interest



Tracks, as a function of time & location:

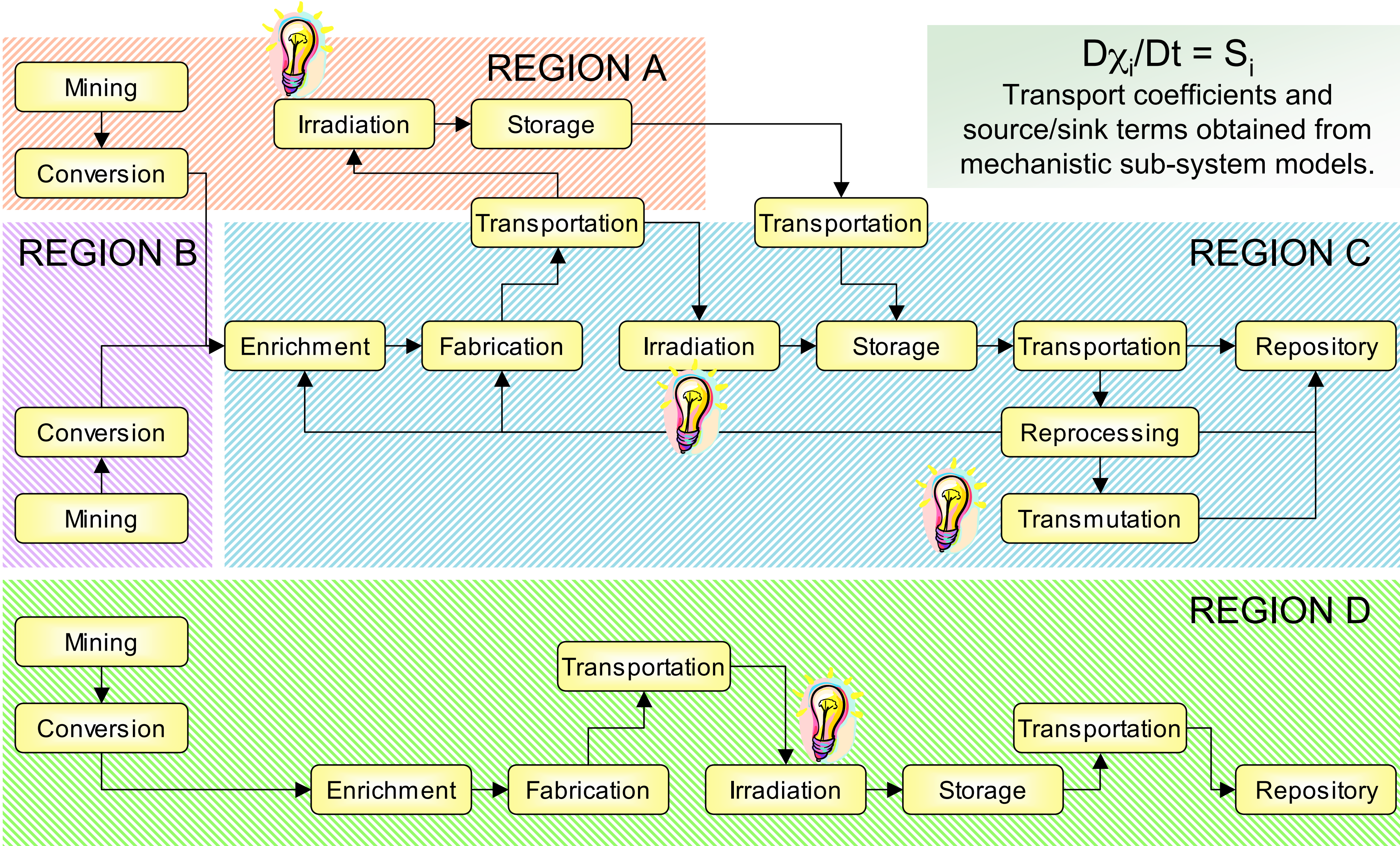
- Raw materials (natural resources)
- Processed materials
- Nuclear materials transportation flow
- Nuclear facilities and their characteristics
- Material storage
- Cost/expenditure/investments
- Products and by-products
  - Electricity
  - Hydrogen
  - Nuclear waste, etc…



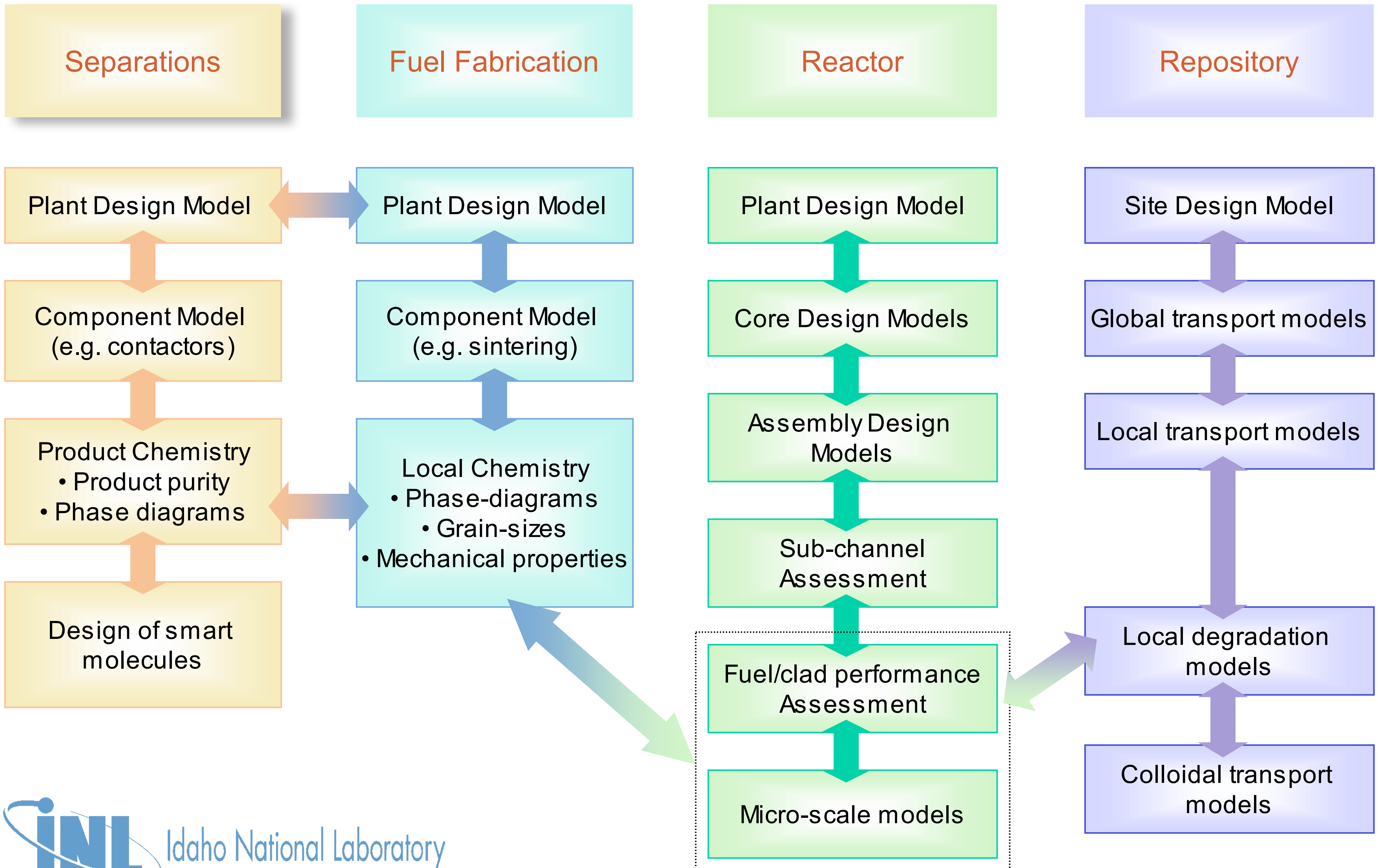
An example would be the assessment of global nuclear materials management under "regional center" concept

$D\chi_i/Dt = S_i$

Transport coefficients and source/sink terms obtained from mechanistic sub-system models.



A layered interactive modeling approach is an effective way to analyze multi-scale phenomenology



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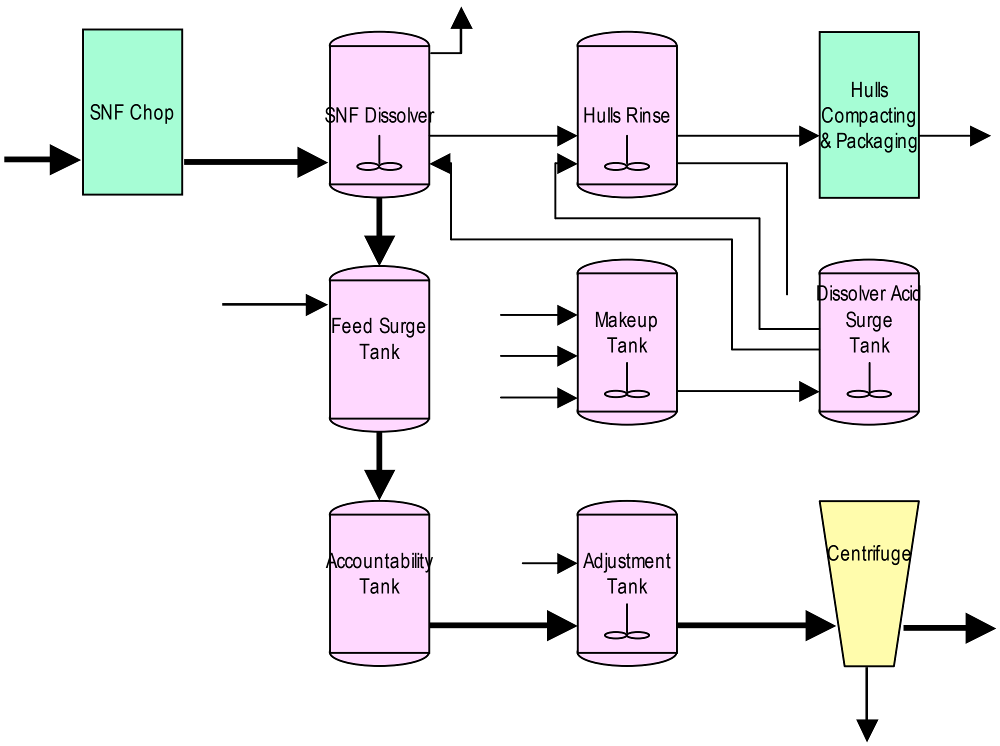
SESAME:
Simulation Enabled Safeguards Assessment MEthodology



Virtual Design of a Separations & Partitioning Plant using “Safeguards by Design”

- Walk-through models and overall system simulation model
- Detailed mechanistic models for plant components
  - Including safeguards instrumentation
  - Control and monitoring system logic (safeguards envelope)
- Plant optimization:
  - Efficiency
  - Advanced safeguards
- Proliferation signatures
  - Design features for detection and/or prevention
- Comparison of various technologies
  - Safeguards efficiency
  - Performance efficiency & cost
- Define the advanced separations plant design for the next generation plants

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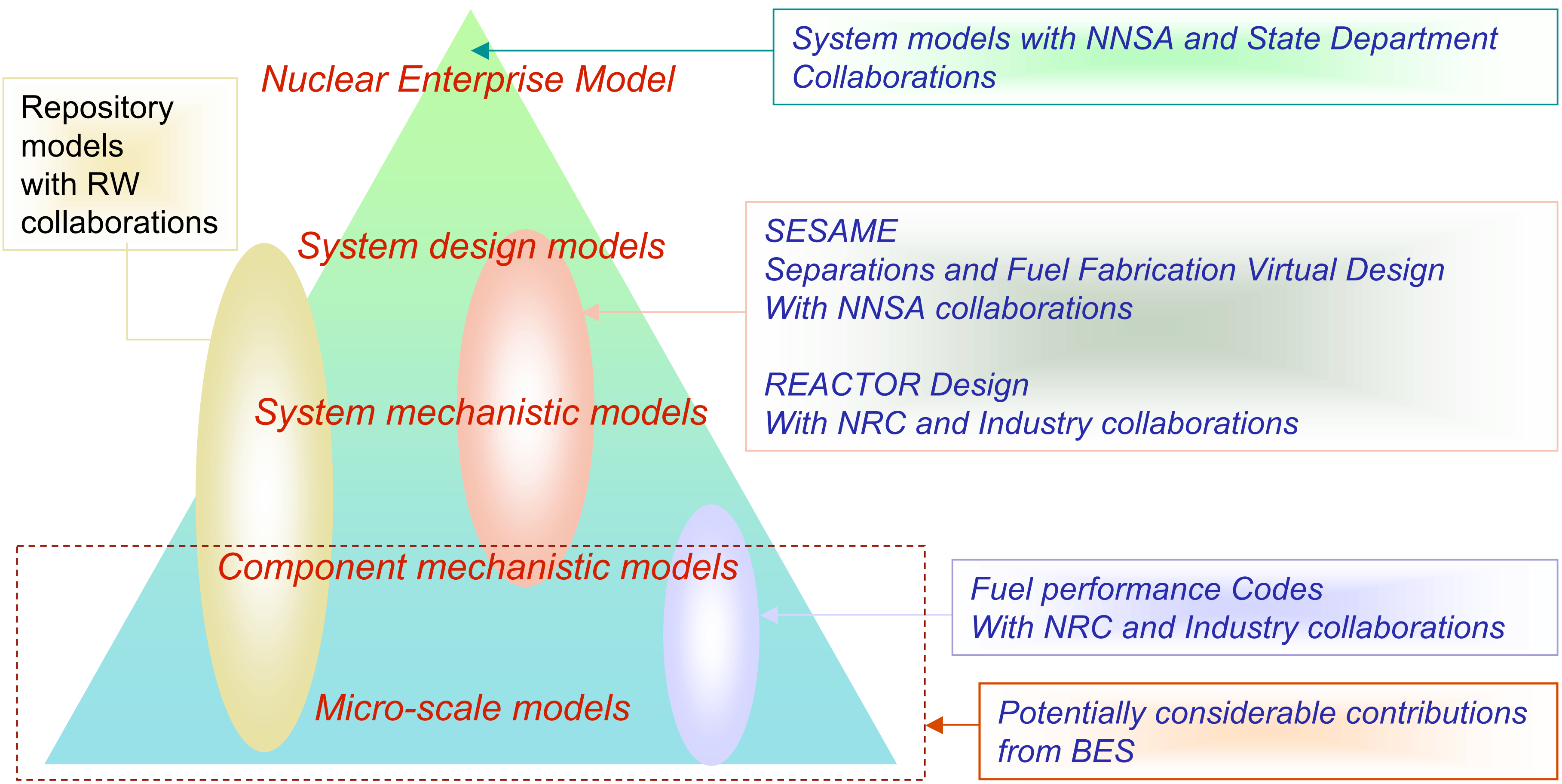
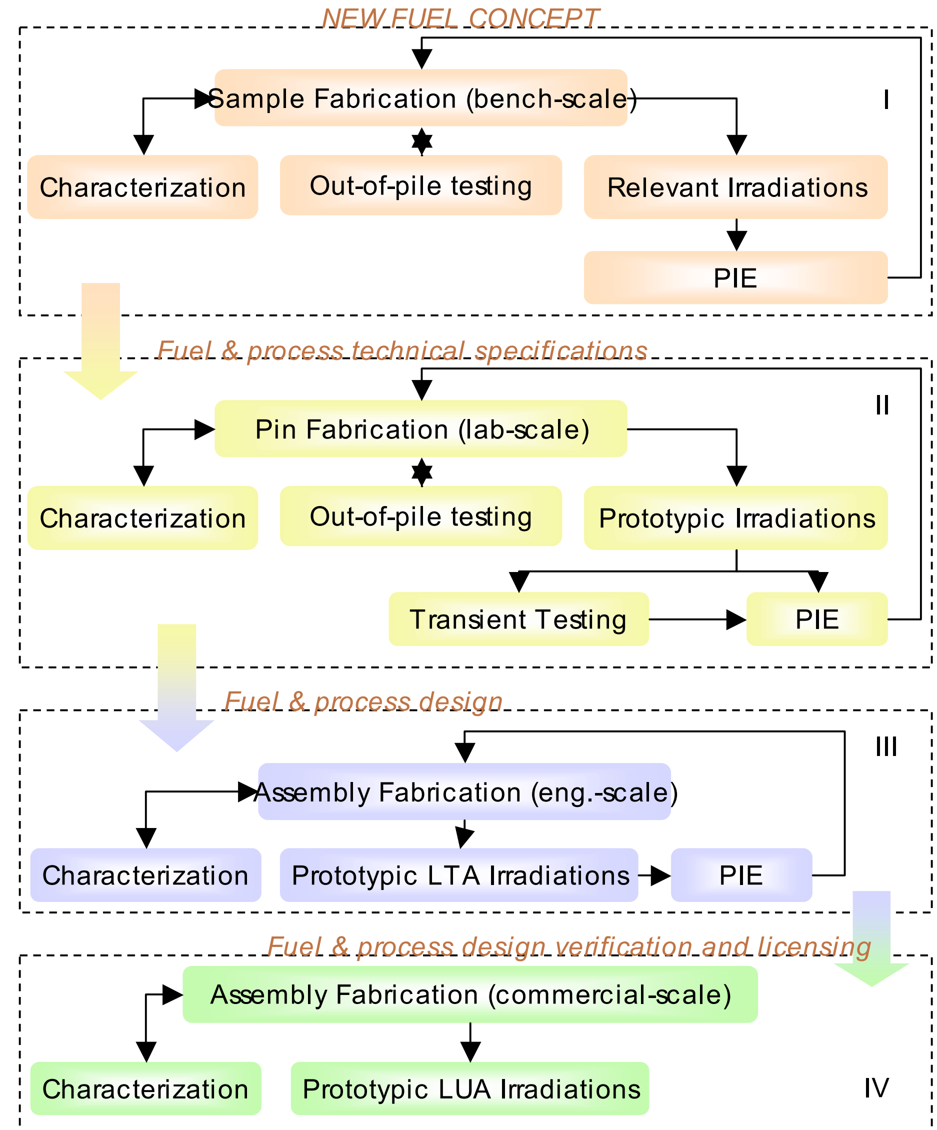
Targeted collaborative projects can be defined within SINEMA and implemented under a consistent framework





FUEL QUALIFICATION

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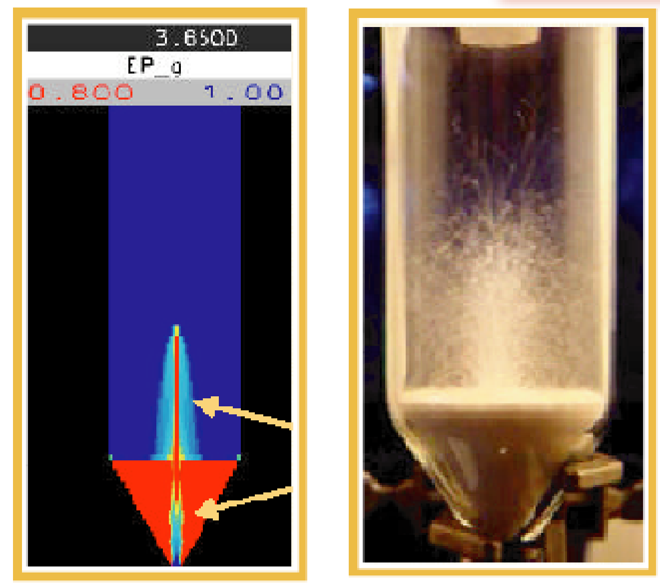
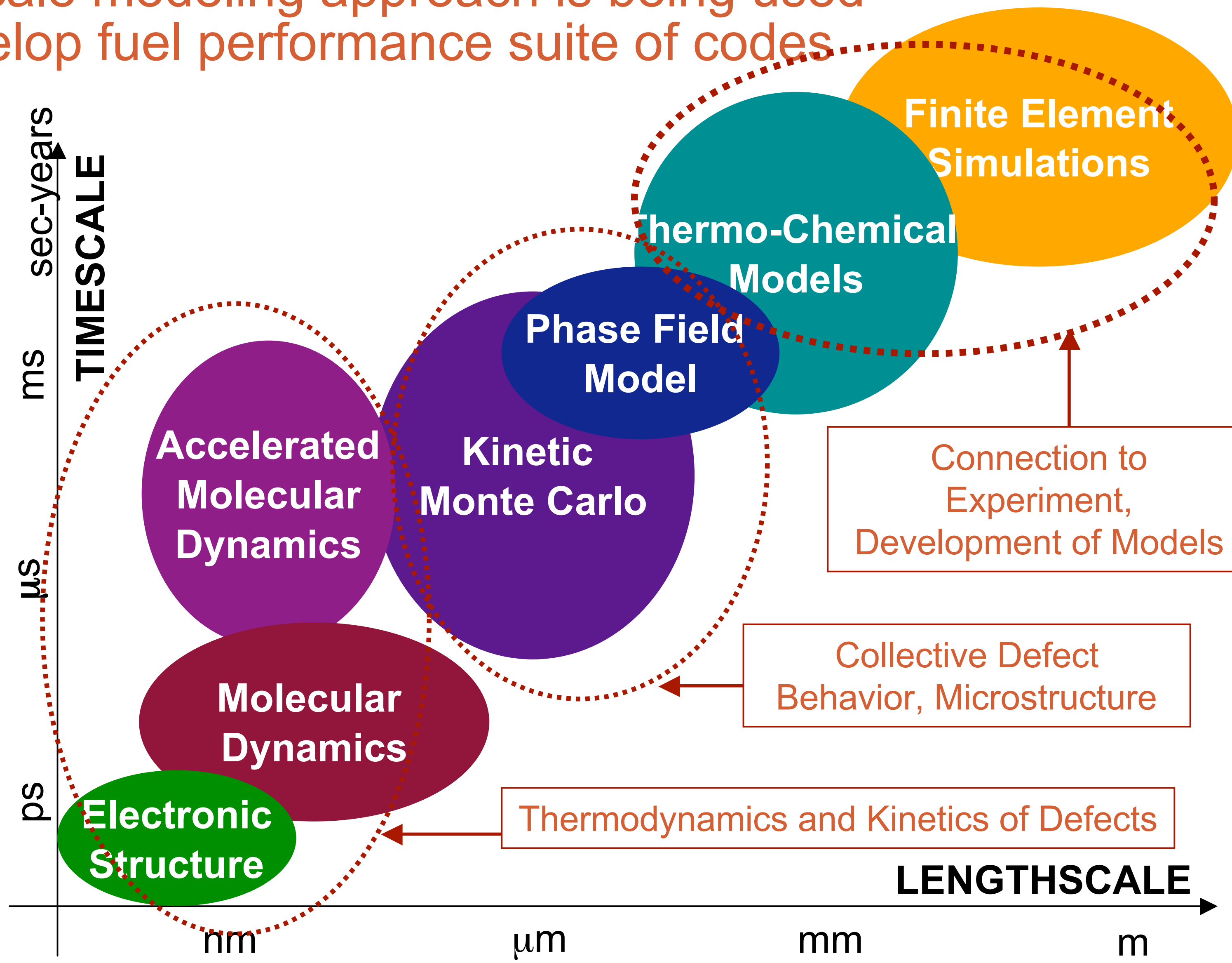
Fundamental understanding of the fuel fabrication processes is key to successful fuel development

Coupled hydraulic-mass transfer-chemistry modeling of TRISO fuel coating process is a good example for the role of advanced modeling in fuel fabrication



At least, an order of magnitude increase in computational speed would enable the tool to have serious impact on the design.

Multi-scale modeling approach is being used do develop fuel performance suite of codes



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Courtesy of Marius Stan (LANL)

The time is right for a major modeling and simulation initiative to complement DOE's nuclear energy initiatives

- In the area of modeling and simulation, nuclear energy has some catching up to do with other similarly capital intensive industries.
- Computational technology is nearly mature to perform large scale modeling and simulation in support of nuclear energy deployment.
  - It is time to take aggressive steps towards an integrated approach
- With a focused effort, we can make substantial contributions in 5 years and revolutionize the nuclear industry in 10 years.
- A SINEMA-like implementation concepts will
  - Focus the modeling and simulation efforts
  - Establish a framework for the overall nuclear energy enterprise effort
    - Focused experiments supported by advanced modeling
  - Provide opportunities for joint projects among National Labs - Regulatory Agencies - Industry - Academia
  - Guide the development of next generation of human resources through strong university participation.